Numerical Simulations of the Flame Front Dynamics by Particles Method within G-equation

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ABSTRACT
The objectives of the present study is the development of effective numerical algorithm to model the flame front evolution in given flow field described by G-equation. The flame front in this model propagates in prescribed flow field with normal to flame front burning velocity depending on the local curvature of the flame front.

1. Introduction

Numerical simulation of gas combustion with detailed chemical kinetics and complex gas flows demands huge computing expenses, therefore there is a necessity to apply more simple, but not losing the physical meaning, the simplified models of flame evolution. When the characteristic scale of internal structure of a combustion wave much less than characteristic size of gas flow perturbations, one can consider flame as an interface between unburned and burned gasses. This model assumes that flame surface moves along its normal with given velocity called a burning velocity. The value of burning velocity can be estimated by preliminary simulation of planar laminar flame taking into account detailed kinetics of chemical reactions. In this approximation the gas flow is determined by equations free of effects introducing by combustion. This approximation is known as “flamelet” model [1] and it is widely used in engineering simulations. In the simplest case, one can assumes that the burning velocity is constant and it is determined by mixture content only. The novelty of the model considered in the paper is that the flame velocity depends on the local curvature of the flame front. An effective algorithm of flame front simulations in the given non-stationary gas flow fields is presented. The algorithm is based on representation of the continuous media as set of a large number of elementary particles, moving on the fixed trajectories, corresponding to the given flow field. The formulation of the model and the algorithm of the calculations is described in the next section.

2. Model

The flame is considered as a surface dividing unburned and burned mixture. This surface moves in unburned mixture with a burning velocity U_b along normal to its surface [2]. Writing the flame front equation in the form $F(x, t) = 0$ and assuming that flame front propagates in the unburned gas with given flow velocity field $V(x, t)$ one can obtain the flame front evolution equation or “G-equation” in the form

$$\frac{\partial F}{\partial t} - \left(\vec{V}, \vec{\nabla F}\right) = U_b \left|\vec{\nabla F}\right| \qquad (1)$$

It is interesting that this equation is similar to the Hamilton-Jacobi equation describing propagation of the relativistic particle [3]. We assume that burning velocity U_b depends on local flame front curvature as follow:

$$U_b = U_b^0(1 + \sigma\kappa) \qquad (2)$$

Here $\kappa = \mathrm{div}(\vec{\nabla F} / \left|\vec{\nabla F}\right|)$ is the flame front curvature and σ is Markstein length [4].

Flame front evolution in the case of resting gas can be described on the base of the Huygens principle applying in the ray optics. Let us suppose that flame front shape is known at some moment, for instance at $t = 0$. In order to find the flame front shape at subsequent time moment $t = dt$ according to the Huygens principle the set of spheres of radius $U_b dt$ with its centers belonging to the initial surface should be plotted. The envelope curve of this set of spheres represents the flame shape. Applying this principle for subsequent time intervals the flame front evolution can be tracked. In the case of the flow field $\vec{V}(\vec{x}, t)$ the technique based on the Huygens principle can be applied too. The only difference is that all points of initial surface must be previously shifted on vector $\vec{V}(\vec{x}, t)\,dt$. Proposed algorithm assumes that continuum is filled by the finite number of randomly distributed particles moving with velocity equal to the local velocity in corresponding 2-D point. Each particle is characterized by spatial coordinates and value describing the state of the corresponding elementary gas volume, namely unburned or burned.

On each time step all unburned particles located inside the circles centered at the burned particles are replaced by the burning particles. The procedure of particles properties changing is applied at every fixed time step τ and the circles radius is $U_b\tau$. To determine the flame front, a third type of particles was introduced called "ignited". These particles have changed their state from not burning to burning during the current iteration in time. The set of ignited particles determines the flame front.

3. Results

This section presents the results of calculating the shape of the flame for the cases of Poiseuille flow and a diverging cylindrical flame. In the case of Poiseuille flow the velocity component along y axes depends on transverse coordinate x only

$$V(x) = V_0\left(1 - \frac{x^2}{L^2}\right) \qquad (3)$$

and the stationary flame front is determined by formula as $F(x,y)=y - f(x)=0$. The results of simulations by proposed particles method and the exact solution by equation (1) are shown in Figure 1. Blue points show the “ignited” particles. The averaged curve constructed by the moving average method exactly coincides with the

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shape of the flame front calculated by formula (1) with constant burning velocity (σ=0).

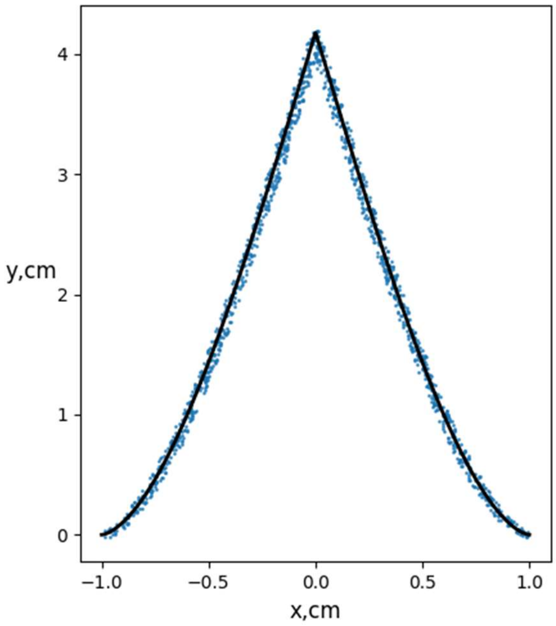

Fig. 1 Flame front shape calculated by particles method and by equation (1) for the case $V_0 = 5U_b$ and L = 1cm. The blue points show the "ignited" particles and the solid curve is flame front shape.

As follows from Figure 1, in the top of flame appears the fracture line according to Huygens-Fresnel principle. Taking into account the effect of flame curvature the flame front in the top of flame becomes smooth. The results of simulations of flame front obtained with and without flame curvature effect are shown in Figure 2.

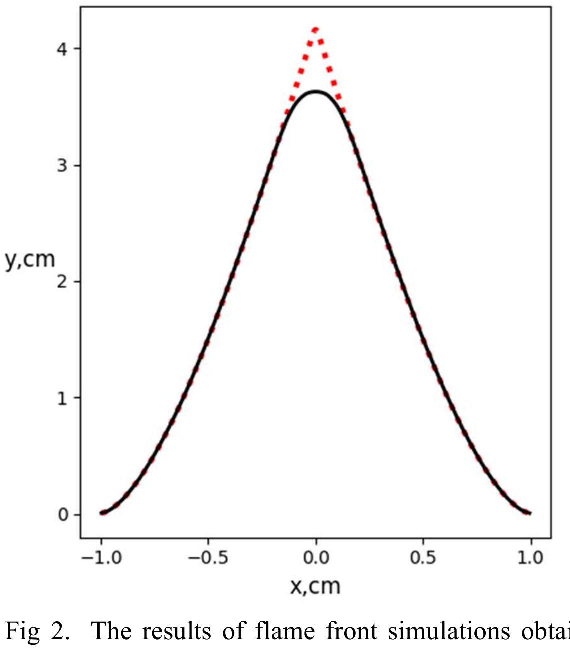

Fig 2. The results of flame front simulations obtained with (solid line) and without (dotted curve) flame curvature effect evaluated for $\sigma = 0.1cm$, $V_0 = 5U_b$ and L = 1cm

The value of the curvature of the front at a point can be obtained from the ratio of the number of burning particles N_b to the total number of particles N' located in the a circle around the point at the front where the flame front curvature is estimated. The local flame front curvature is determined by formula

$$\kappa = 0.5 - \frac{N_b}{N'} \quad (4)$$

In the case of equal numbers of burned and unburned particles inside the circle ($N_b = N'/2$) the curvature is zero. If there number of burning particles is less number of unburned particles, then the curvature is positive, and if vice versa, then negative. This method allows fast calculation of local flame front curvature at any point of calculated domain irrespective to orientation of the flame front with respect of the coordinate system. The effect of curvature on the dynamics of flame propagation is clearly demonstrated by calculations of a diverging cylindrical flame velocity. In the absence of curvature effects, the dimensionless radial velocity of the flame is constant and equal to unity. Taking into account the effects of curvature, the speed depends on the radius according to formula (2). This case allows verification of calculations performed by the particle method.

4. Discussion

In the paper the numerical algorithm describing flame front evolution within frame of "flamelet" model is suggested. This algorithm assumes the representation of the continuous medium by set of discrete particles. The developed algorithm can be generalized in future to the model that takes into account self-ignition and flame quenching mechanism. For this aim one can apply the flame front model that incorporates flame front inertial effects [5].

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